

Conductance of a double quantum dot with correlation-induced wave function renormalization

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Abstract

The zero-temperature conductance of diatomic molecule, modelled as a correlated double quantum dot attached to noninteracting leads is investigated. We utilize the Rejec-Ramšak formulas, relating the linear-response conductance to the ground-state energy dependence on magnetic flux within the framework of EDABI method, which combines exact diagonalization with *ab initio* calculations. The single-particle basis renormalization leads to a strong particle-hole asymmetry, of the conductance spectrum, absent in a standard parametrized model study. We also show, that the coupling to leads $V \approx 0.5t$ (t is the hopping integral) may provide the possibility for interatomic distance manipulation due to the molecule instability.

Key words: Correlated nanosystems, Conductance, EDABI method

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Recent progress in nanotechnology made possible to fabricate small systems attached to leads, and to measure the conductance of even a single hydrogen molecule [1]. In such systems strong electron correlations can play a decisive role [2]. The theoretical understanding of the experiments is far from complete, partly because the nanoscale leads geometry often introduces a degree of irreproducibility, and partly due to many body effects on the intrinsic transport properties of such single-molecule devices. In particular, the electron-phonon coupling was recently shown shrink the conductance peak for a single quantum dot in a Kondo regime [3], since the on-site Coulomb repulsion U is effectively renormalized in a system ground state. Here we describe a qualitatively similar effect in a double quantum dot, produced solely by electron-electron interaction only through a completely different physical mechanism: the correlation-induced wave-function renormalization [4].

We start with the Hamiltonian which is a generalization of the Anderson impurity model [5], and can be written as

$$H = H_L + V_L + H_C + V_R + H_R, \quad (1)$$

where H_C models the central region, $H_{L(R)}$ describes the left (right) lead, and $V_{L(R)}$ is the coupling between the lead and the central region. Both $H_{L(R)}$ and $V_{L(R)}$ terms have

a tight-binding form, with the hopping t and the tunneling amplitude V , as depicted schematically in Fig. 1. The central-region Hamiltonian H_C describes a double quantum dot with electron-electron interaction, and has a form

$$H_C = (\epsilon_a - eV_G) \sum_{j=1,2} n_j - t' \sum_{\sigma=\uparrow,\downarrow} (c_{1\sigma}^\dagger c_{2\sigma} + \text{h.c.}) + U \sum_{j=1,2} n_{j\uparrow} n_{j\downarrow} + K n_1 n_2 + (Ze)^2/R, \quad (2)$$

where ϵ_a is atomic energy, V_G is an external gate voltage, t' is the internal hopping integral, U and K represents the intra- and inter-site Coulomb interactions, respectively, and the last term describes the Coulomb repulsion of the two ions at the distance R . Here we put $Z = 1$ and calculate all the parameters ϵ_a , t' , U , and K as the Slater integrals [6] for $1s$ -like hydrogenic orbitals $\Psi_{1s}(\mathbf{r}) = \sqrt{\alpha^3/\pi} \exp(-\alpha|\mathbf{r}|)$, where α^{-1} is the orbital size (*cf.* Fig. 1). The parameter α is optimized to get a minimal ground state energy for

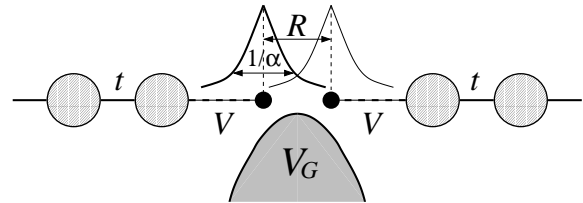


Fig. 1. Diatomic molecule as a double quantum dot.

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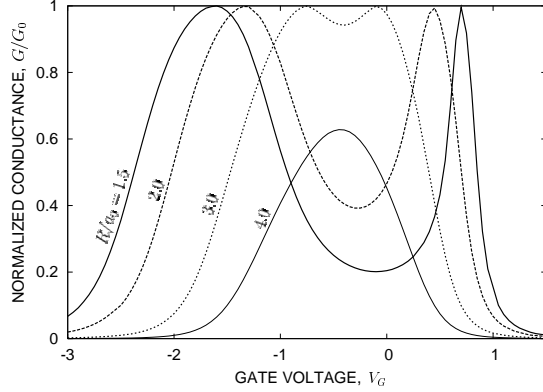


Fig. 2. Zero-temperature conductance of the system in Fig. 1 as a function of the gate voltage V_G and interatomic distance R . $1s$ orbital size α^{-1} is optimized variationally. The lead parameters are $t = 1\text{Ry}$ and $V = 0.5t$.

whole the system described by the Hamiltonian (1). Thus, following the idea of EDABI method [7], we reduce the number of physical parameters of the problem to just a three: the interatomic distance R , the gate voltage V_G , and the lead-molecule coupling V (we put the lead hopping $t = 1\text{Ry} = 13.6\text{eV}$ to work in the wide-bandwidth limit).

We discuss now the molecule conductivity calculated from the Rejec-Ramšak two-point formula [8]:

$$G = G_0 \sin^2 \pi [E(\pi) - E(0)] / 2\Delta, \quad (3)$$

where $G_0 = 2e^2/\hbar$ is the conductance quantum, $\Delta = 1/N\rho(\epsilon_F)$ is the average level spacing at Fermi energy, determined by the density of states in an infinite lead $\rho(\epsilon_F)$, $E(\pi)$ and $E(0)$ are the ground-state energies of the system with periodic and antiperiodic boundary conditions, respectively. $E(\phi)$ is calculated for $\phi = 0, \pi$ within the Rejec-Ramšak variational method [8], complemented by the inverse orbital size α optimization, as mentioned above. We use typically $N = 10^2 \div 10^3$ sites to reach the convergence.

In Fig. 2 we show the conductivity for $V = 0.5t$, and different values of the interatomic distance R . The conductance spectrum evolves from the situation well-separated peaks corresponding to the independent filling of bonding and antibonding molecular orbitals ($R \lesssim 2a_0$, where a_0 is the Bohr radius), to the single peak in the intermediate range ($R \approx 3a_0$), which decays when $t' \ll V$ for large R .

Probably, the most interesting feature of the spectra depicted in Fig. 2 is their strong asymmetry for small R . Namely, the low- V_G conductance peak, corresponding to the system filling $\langle n_1 + n_2 \rangle \approx 1$ (one *hole*) is significantly wider than the high- V_G peak for $\langle n_1 + n_2 \rangle \approx 3$ (one *extra electron*). Such a particle-hole symmetry breaking is the novel feature, observed when including the correlation-induced basis optimization, and absent in the parametrized-model approach [8,9]. It is also a new feature of a nanosystem, do not observed in mesoscopic double quantum dots [10], where the particle-hole symmetry is perfect.

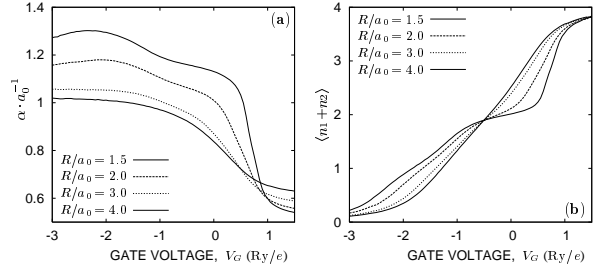


Fig. 3. The optimized inverse orbital size (a) and average central region occupancy (b) for the diatomic molecule attached to noninteracting leads characterized by the parameters $t = 1\text{Ry}$ and $V = 0.5t$.

The relation between the observed asymmetry, basis renormalization, and electron correlations can be clarified as follows. *First*, one can observe that the optimal values of the variational parameter α , provided in Fig. 3a, decrease dramatically for high V_G , corresponding to the overdoped situation $\langle n_1 + n_2 \rangle > 2$ (cf. Fig. 3b). This is because the system minimize energy of double occupancies, which is of the order $U \sim \alpha$ [6]. *Then*, we focus on a small R limit, in which the well separation of molecular orbitals allows one to approximate the expression for a single impurity at zero temperature [11]

$$G = G_0 \sin^2(\pi \langle n_k \rangle / 2), \quad (4)$$

where $\langle n_k \rangle$ is the bonding ($k = 0$) or antibonding ($k = \pi$) orbital occupancy. Expanding around the maximum we have $G(V_G) - G(V_G^{*,k}) \approx -G_0(\chi_c \pi / 2)^2 (V_G - V_G^{*,k})^2$, where $V_G^{*,k}$ ($k = 0, \pi$) is the low/high voltage peak position and χ_c is the charge susceptibility, which may be approximated as $\chi_c \approx \partial \langle n_1 + n_2 \rangle / \partial V_G$, since the orbitals are filled separately. Values of the later derivative read from Fig. 3b around the low and high voltage peak positions ($\langle n_1 + n_2 \rangle \approx 1$ and ≈ 3 , respectively) provides a clear asymmetry. Moreover, the expansion of $G(V_G)$ allows one to roughly estimate the peak width as $\Delta V_G \approx \chi_c^{-1} \approx (U + K)/2 \sim \alpha$, what provides an indirect correspondence between the spectrum asymmetry and basis renormalization.

The practical possibility of the conductance measurement involving atoms manipulation (changing of R) were also explored in terms of the system stability. Namely, the binding energies $\Delta E \equiv E_{R_{\min}} - E_\infty$ (where R_{\min} is the bond length), listed in Table 1, shows that the system become metastable around $V = 0.5t$ ($\Delta E > 0$ indicates a *local* en-

Table 1

The binding energy ΔE and the bond length R_{\min} for different coupling to the lead V . The conductance at the energy minimum is also provided.

V/t	ΔE	R_{\min}/a_0	$G_{\min}^{V_G=0}/G_0$
0.0	-0.296	1.43	0
0.1	-0.293	1.44	10^{-4}
0.2	-0.282	1.46	0.004
0.3	-0.180	1.52	0.023
0.4	-0.040	1.59	0.093
0.5	+0.074	1.93	0.422

ergy minimum). Therefore, the binding of the atoms to the lead become stronger than interaction between the atoms, that may allow individual atoms manipulation.

In *summary*, we have supplemented the double quantum dot conductance calculation with the single-particle basis optimization. Apart from simplifying the analysis, such an approach leads to substantially new physical effects, since it breaks the particle-hole symmetry of the Hamiltonian.

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References

- [1] R.H.M. Smit *et al.*, *Nature* **419**, 906 (2002);
- [2] W. Liang *et al.*, *Nature* **417**, 725 (2002).
- [3] P. S. Cornaglia *et al.*, *Phys. Rev. Lett.* **93**, 147201 (2004).
- [4] J. Spalek *et al.*, *Phys. Rev. B* **61**, 15676 (2000); *Acta Phys. Polon. B* **31**, 2879 (2000); *ibid.* **32**, 3189 (2001).
- [5] P. W. Anderson, *Phys. Rev.* **124**, 41 (1961).
- [6] J. C. Slater, *Quantum Theory of Molecules and Solids*, McGraw-Kill (New York, 1963), Vol. 1, p. 50; J. Spalek *et al.*, Ref. [4].
- [7] A. Rycerz, J. Spalek, *Eur. Phys. J. B* **40**, 153 (2004); *Phys. Rev. B* **63**, 073101 (2001); *ibid.* **65**, 035110 (2002).
- [8] T. Rejec, A. Ramšak, *Phys. Rev. B* **68**, 035342 (2003); *ibid.* 033306.
- [9] T. Kostyrko, B. Bulka, *Phys. Rev. B* **67**, 205331 (2003).
- [10] W. G. van der Wiel *et al.*, *Rev. Mod. Phys.* **75**, 1 (2003).
- [11] Y. Meir, N. S. Wingreen, *Phys. Rev. Lett.* **68**, 2512 (1992); H. M. Pastawski, *Phys. Rev. B* **46**, 4053 (1992). A.-P. Jauho, N. S. Wingreen, Y. Meir, *ibid.* **50**, 5528 (1994).